Calculation A. Sample calculation from concentration in soil-vapor to concentration in soil¹

1. Converting parts per billion by volume to micrograms per cubic meter (ADEQ, 2008a).

$$\frac{\mu g}{m^3} = ppbv \times \frac{MW}{24.45}$$

Where MW is Molecular weight in grams per mole (g/mole) and 24.45 is at standard temperature and pressure (25°C and 1 atmosphere).

Using 200,00 ppbv from the measured concentration of TCE and 131.4 g/mole for the molecular weight of TCE (CDC, 2010) gives

$$\frac{\mu g}{m^3} = 200,000 \ ppbv \times \frac{131.4 \ g}{24.45} = 1074764.83 \ \frac{\mu g}{m^3}$$

2. Converting micrograms per cubic meter to micrograms per liter

$$\frac{\mu g}{L} = \frac{\mu g}{m^3} \times \frac{1 \ m^3}{1,000 \ L}$$

Using the calculated concentration in µg/m³ gives

$$\frac{\mu g}{L} = 1074764.83 \frac{\mu g}{m^3} \times \frac{1 m^3}{1,000 L} = 1074.76 \frac{\mu g}{L}$$

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¹ Sample Taken from MM-80-10 on May 23, 2002 for Trichlororethene (TCE).

3. Using micrograms per liters to get the concentration in soil in micrograms per kilogram using the linear sorption portioning equation and Henry's Law (ADEQ, 2008a).

$$C_t = \frac{C_g \left[\frac{K_{OC} f_{OC} \rho_b}{H_O} + \frac{\theta_w}{H_O} + (\theta_t - \theta_w) \right]}{\rho_b}$$

 C_t = total concentration in soil ($\mu g/kg$)

 C_g = concentration in soil vapor ($\mu g/L$)

K_{oc}=soil organic carbon-water partitioning coefficient (L/kg)=166 L/kg (ADEQ, 2008a)

f_{oc} = fraction of organic carbon (g-organic carbon/g-soil)= 0.006 (ADEQ, 2008a)

 ρ_b =dry bulk density (kg/L) = 1.5 kg/L (ADEQ,2008a)

H_o = Henry's law Constant (dimensionless)=0.422 (ADEQ,2008a)

 $\theta_{\rm w}$ = volumetric water content (volume of water/volume of soil) = 0.15 (ADEQ, 2008a)

 θ_t = total soil porosity (volume of voids/volume total) = 0.43 (ADEQ, 2008a)

Using the number stated above and the calculated concentration in soil vapor in µg/L gives

$$C_{t} = \frac{1074.76 \frac{\mu g}{L} \left[\frac{166 \frac{L}{kg} \cdot 0.006 \cdot 1.5 \frac{kg}{L}}{0.422} + \frac{0.15}{0.422} + (0.43 - 0.15) \right]}{1.5 \frac{kg}{L}} = 2991.96 \frac{\mu g}{kg}$$

4. Converting micrograms per kilogram to milligrams per kilogram

$$\frac{mg}{kg} = \frac{\mu g}{kg} \times \frac{1 \, mg}{1,000 \, \mu g}$$

Using the calculated concentration in soil in µg/kg gives

$$\frac{mg}{kg} = 2991.96 \frac{\mu g}{kg} \times \frac{1 mg}{1,000 \mu g} = 2.992 \frac{mg}{kg}$$

Calculation B. Calculating soil-gas and water concentrations through Henry's Law

- a. Soil-Vapor to Water Concentration
- 1. Putting ppbv into mole fraction form. Because ppbv is already a fraction, dividing by a billion will give the simplified mole fraction.

$$\frac{200,000\ ppbv}{10^9} = 0.0002$$

2. Using Raoult's Law to convert mole fraction to partial pressure. The total pressure was assumed to be at standard pressure, 1 atmosphere (atm).

$$p_A = y_A P$$

p_A: Partial Pressure of A

y_A: Mole Fraction of A in gas phase

P: Total pressure of system

$$p_A = 0.002 \cdot atm = 0.002 atm$$

3. Using Henry's Law Constant (Watts, 1997) to convert partial pressure to a concentration in water.

Henry's Law Constant states

$$P = H \cdot X$$

P=Partial pressure

H= Henry's Law Constant

X= Concentration of compound in water

Rearranging to solve for X gives

$$X = \frac{P}{H}$$

Plugging in the calculated partial pressure and Henry's Constant of 9.1 \times 10⁻³ $\frac{atm \cdot m^3}{mole}$ (Watts, 1997) gives

$$X = \frac{0.002 \ atm}{9.1 \times 10^{-3} \ \frac{atm \cdot m^3}{mole}} = 0.021978 \ \frac{mole}{m^3}$$

4. Converting mole/m³ to mole/L

0.021978
$$\frac{mole}{m^3} \cdot \frac{1 m^3}{1,000 L} = 2.2 \times 10^{-5} \frac{mole}{L}$$

5. Converting mole/L to μg/L

$$2.2 \times 10^{-5} \frac{mole}{L} \cdot MW \cdot \frac{1 \, \mu g}{10^{-6} g}$$

MW= Molecular weight of TCE, 131.4 g/mol (NIOSH)

Plugging in MW gives

$$2.2 \times 10^{-5} \frac{mole}{L} \cdot 131.4 \frac{g}{mole} \cdot \frac{1 \mu g}{10^{-6} g} = 2887.91 \frac{\mu g}{L}$$

- b. Converting concentration in water to soil-gas data
 - 1. Converting μg/L to mole/L

$$5100 \frac{\mu g}{L} \cdot \frac{1}{MW} \cdot \frac{10^{-6}g}{1 \mu g}$$

MW= Molecular weight of TCE, 131.4 g/mol (NIOSH)

Plugging in MW gives

$$5100 \frac{\mu g}{L} \cdot \frac{1 \ mole}{131.4 \ g} \cdot \frac{10^{-6} g}{1 \ \mu g} = 3.9 \times 10^{-5} \frac{mole}{L}$$

2. Converting mole/L to mole/m³

$$3.9 \times 10^{-5} \frac{mole}{L} \cdot \frac{1,000 L}{1 m^3} = 0.038813 \frac{mole}{m^3}$$

3. Using Henry's Law Constant (Watts, 1997) to convert a concentration in water to a partial pressure.

Henry's Law Constant states

$$P = H \cdot X$$

P=Partial pressure

H= Henry's Law Constant

X= Concentration of compound in water

Plugging in the calculated concentration and Henry's Constant of 9.1 \times 10⁻³ $\frac{atm \cdot m^3}{mole}$ (Watts, 1997) gives

$$P = 9.1 \times 10^{-3} \frac{atm \cdot m^3}{mole} \cdot 0.038813 \frac{mole}{m^3} = 3.53 \times 10^{-4} atm$$

4. Using Raoult's Law to convert partial pressure to mole fraction. The total pressure was assumed to be at standard pressure, 1 atmosphere (atm).

$$p_A = y_A P$$

p_A: Partial Pressure of A

y_A: Mole Fraction of A in gas phase

P: Total pressure of system

Rearranging to solve for the mole fraction gives

$$y_A = \frac{p_A}{P}$$

Plugging in the calculated partial pressure and assumed total pressure gives

$$y_A = \frac{3.53 \times 10^{-4} \ atm}{1 \ atm} = 3.53 \times 10^{-4}$$

5. Putting the mole fraction into ppbv form. Multiplying the mole fraction by a billion will give the ppbv.

$$3.53 \times 10^{-4} \cdot 10^9 = 353,196 \ ppbv$$